Computational Science and Engineering
Charter Renewal

This CHARTER RENEWAL applies to the SIAM Activity Group on Computational Science and Engineering. The SIAM Activity Group (or SIAG) to which this renewal applies was originally formed under the aegis of SIAM on December 15, 2000 by the SIAM Council and December 2, 2000 by the SIAM Board of Trustees with its initial operating period beginning January 1, 2001 and ending December 31, 2003. Its charter has been renewed by the Council and Board seven times thereafter. This SIAG has 2013 members, including 884 student members, as of December 31, 2013.

According to its Rules of Procedure, the objective(s) of the SIAM Activity Group on Computational Science and Engineering are to:

- foster collaborations among applied mathematicians, computer scientists, domain scientists and engineers in those areas of research related to the theory, development, and use of computational technologies for the solution of problems in science and engineering.
- promote and facilitate Computational Science and Engineering as an academic discipline.
- promote computational simulation as a peer to theory and experiment in the process of scientific discovery.

Within the framework of SIAM, the SIAG will conduct activities that implement its purposes.
Its proposed functions are:

1) Organize minisymposia at the SIAM Annual Meeting on years where there is no SIAG conference.

2) Organize a track of at least six minisymposia at the SIAM Annual Meeting at least once every five years. The VP for Programs and the VP at Large will coordinate the scheduling with the SIAG Chair.

Other activities can include:

3) Organize a biennial SIAM Conference on computational science and engineering. The SIAG will consider dovetailing specialized workshops and conferences with the SIAM Annual Meeting or other SIAG conferences. The Chair of the Conference Organizing Committee shall be either the Program Director or the Chair of the SIAG or their designee. The organizing committee must be approved by the VP for Programs at least 16 months before the conference.

4) With the approval of the SIAM Program Committee, the SIAG may organize special sessions at SIAM meetings, and conduct special one- or two-day meetings immediately before or after a regular SIAM meeting. Other SIAG meetings may be organized only with the approval of the SIAM President and Vice President for Programs.

5) Broker partnerships between academia, industry, and government laboratories. The SIAG will seek to facilitate the establishment of academic programs in CS&E to foster its development as an academic discipline. The SIAG also will facilitate the placement of undergraduate and graduate students in internships in industry and government laboratories.

6) Work with other societies to promote CS&E. The SIAG will work with other professional societies to promote CS&E. For example, SIAM and another society might organize a workshop on a topic of mutual interest. The SIAG also would attempt to increase government support for CS&E through various outreach activities.

7) Disseminate information. The SIAG may publish a newsletter, offer a members' list serve or maintain a Website to facilitate the exchange of information among its members and other interested parties.

8) SIAM/ACM Prize in Computational Science and Engineering (with ACM):
The SIAM/ACM Prize in Computational Science and Engineering, established in 2002, is awarded by the Society for Industrial and Applied Mathematics (SIAM) and the Association for Computing Machinery (ACM) in the area of computational science in recognition of outstanding contributions to the development and use of mathematical and computational tools and methods for the solution of science and engineering problems. This prize is awarded at the biennial SIAM Conference on Computational Science and Engineering.

SIAG meetings, workshops, and conferences may be organized only with the approval of the SIAM President and the SIAM Vice President for Programs.

The SIAG has complemented SIAM's activities and supported its proposed functions. The answers to the questions below indicate how this was accomplished and what the officers propose as the future directions for the SIAG.

1. List all current officers of the activity group (including advisory board, if relevant).

- Chair: Ulrich Ruede, University of Erlangen-Nuremberg, Germany (1/1/2013 - 12/31/2014)
- Vice Chair: Karen Willcox, MIT, USA (1/1/2013 - 12/31/2014)
- Program Director: Lois Curfman McInnes, Argonne National Laboratory, USA (1/1/2013 - 12/31/2014)
- Secretary/Treasurer: Hans De Sterck, University of Waterloo, Canada (1/1/2013 - 12/31/2014)

2. How is the field covered by the activity group doing? Is it growing, is the focus shifting? What have been the significant advances over the last three years?

During the past two decades, large-scale computing has become a prevalent means of discovery, design, and development in almost all areas of research and technology. Computational Science and Engineering (CSE) is playing a central role in this evolution, having established itself as the third pillar of the scientific enterprise alongside theory and physical experiment. The field is strong and growing; in addition, a combination of disruptive developments are redefining the scope and reach of the CSE endeavor. Disruptive developments that have impacted the CSE field include a dramatic growth in computational power and the advent of big data. What was considered supercomputing capability in the 1990s is now the power of a modern laptop. Another challenge and opportunity is the significant

broadening of the application fields of CSE. Examples of fields with an increasing footprint in CSE include biology, quantum chemistry and the geological sciences.

During the last two decades, several universities in the US and abroad have started graduate and undergraduate programs in CSE. These interdisciplinary programs are currently quite diverse. The SIAG has played an important role in defining the setup and the curricula of these programs by providing a template in the form of the SIAM report on "Graduate Education for Computational Science and Engineering," Petzold et al., 2001 (see http://dx.doi.org/10.1137/S0036144500379745). Minisymposia on education in CSE have been held regularly at the SIAM CSE conferences to provide a forum for discussion and exchange of experiences.

3. How is the activity group doing? Is it remaining vibrant? Is the size of the SIAG stable or increasing? How is the SIAG keeping up with the changes in the field? How are the broader interests of SIAM reflected in the activities of the SIAG?

Non-student membership in the SIAG increased by 10% from 1026 members in 2011 to 1129 members in 2013; student membership decreased from 1333 (57% of SIAG members) in 2011 to 884 (44% of SIAG members) in 2013. About 68% of non-student members are from academia, while over 15% of non-student members are from government, and 12% are from industry. Overall female membership (students and non-students) is about 14%.

One of the main activities of the SIAG is the biennial CSE conference. Through this highly active conference we keep the SIAG current to trends in the field and help foster newly emerging areas. For example, at the SIAM CSE13 conference, the invited speakers brought a range of expertise in a vast number of applications areas, from multiscale and multiphysics simulations in science, engineering, and industry to big data and extreme-scale architectures. The conference remains attractive to the membership because it invites a broad range of participation, while focusing on the advancements and impact of CSE. The attendees can showcase their work in a variety of related areas that would otherwise not interact, and they are able to see new ideas in new areas at the forefront of CSE. A variety of events planned for the CSE15 conference target students and early-career researchers, including a job fair, a career panel, minitutorials, and an expanded poster session.

SIAM strengthens the interactions among mathematics, science, and technology. The CSE SIAG is an excellent forum for these interactions, particularly through its conference series. In the past several years, we have strived to maintain a balance on the organizing committees with applied mathematicians, computer scientists, and application scientists. This has been valuable in reaching out to different communities and ensuring the multidisciplinary nature of the SIAG.

4. Please list conferences/workshops the activity group has sponsored or co-sponsored over the past three years, and give a brief (one sentence or phrase) indication of the success or problems with each.

The SIAG/CSE organizes the biennial conference on Computational Science and Engineering. This list of conferences may be found at: http://www.siam.org/meetings/archives.php#CS.

The SIAM Conference on Computational Science and Engineering in 2013 (CSE13) had 1344 attendees. This attendance made CSE13 the largest SIAM conference held to date, with a 65% increase over CSE11 and a four-fold increase in attendance since the first CSE conference in 2000. CSE13 saw an enormous diversity of topics across computational science and engineering. Popular themes among the 270 minisymposia included methods for multiscale and multiphysics problems, numerical methods for PDEs, high performance computing, scientific software, fast algorithms, numerical linear algebra, model reduction, uncertainty quantification, optimization, inverse problems, and CSE education. The poster session saw 61 posters ranging across a similar set of themes. Two special themes of the conference were Big Data and Computational Mathematics for Planet Earth. These special themes were chosen to reflect the designation of 2012 as a special year of emphasis on Mathematics, Statistics, and the Data Deluge, and 2013 as a special year of emphasis on the mathematics of Planet Earth.

As major initiative to explore future CSE directions, the SIAG officers are organizing a workshop on *Future Directions in CSE Education and Research*, to be held August 4-6, 2014, in Breckenridge, Colorado, USA. This invitation-only workshop, sponsored by SIAM and the European Exascale Software Initiative (EESI), will focus on future directions in CSE education and research in light of recent advances in high-performance computing and CSE application areas. The workshop will bring together leaders in the CSE field to update the SIAM report on "Graduate Education for Computational Science and Engineering," Petzold et al., 2001 (see http://dx.doi.org/10.1137/S0036144500379745). Workshop discussions will include possible new strategies and new directions for the CSE discipline -- both in education and in research -- in light of new disruptive developments that include extreme-scale challenges, big data/big computing, and a significant broadening of the application fields of CSE and that are redefining the scope and reach of the CSE endeavor. An outcome of the workshop will be a consolidated compact document of approximately 20-30 pages. As a first step in collecting material, participants were requested to submit a two-page position paper prior to the meeting. We anticipate that the outcomes of this workshop will guide the further development of the CSE field and the SIAG's focus and activities over the coming decade.

5. Please indicate the number of minisymposia directly organized by the activity group at the last two SIAM annual meetings. When did the SIAG last organize a track at an annual meeting or meet jointly with the SIAM Annual Meeting?

The SIAG is organizing a track at the 2014 Annual Meeting with the following minisymposia:

- *Towards Exascale Geophysical Flow Computations* (2 sessions) (organizers Omar Ghattas, Björn Gmeiner, Christian Waluga, Ulrich Rüde)
- *High-Performance Algorithms for Functions of Matrices* (organizers Edvin Deadman, Sivan A. Toledo)
- *Inverse Problems for Coastal Engineering and Subsurface Flow* (organizer Donald Estep)
- *Opportunities in Applied Mathematics Research for Exascale Computing* (organizers Jeffrey A. Hittinger, Karen I. Pao, Jack J. Dongarra)

6. Please indicate other activities sponsored by the activity group, to include newsletters, prizes and web sites. Have each of these been active and successful?

The other activities sponsored by the activity group include the CSE mailing list, a SIAG Wiki, and articles in SIAM News and SIAM Review.

- **CSE Mailing List.** The CSE mailing list is open to all SIAG members who are automatically subscribed when they join the SIAG. We encourage the following types of postings to the mailing list: solicitations for SIAG/CSE sponsored conferences, announcements of CSE-related conferences/events, calls for nominations of prizes, new technical reports, papers, software, open positions, and SIAM announcements such as electronic publication, general conference announcements and other news. The list is fully moderated in order to prevent redundant or inappropriate posts. Information on the list can be found at http://lists.siam.org/mailman/listinfo/siam-cse .

- **SIAG Wiki.** The CSE SIAG established a Wiki where information relevant to the field can easily be exchanged. Appropriate material for posting includes listings of upcoming meetings of interest to the field, presentation slides from CSE meetings, links to external relevant pages, business meeting notes, etc.

- **SIAM News.** The following SIAM News articles (coordinated by G. Corbett, L.C. McInnes and K. Willcox) covered topics of the CSE13 Conference:
  - CSE 2013: "Big Data" and "Planet Earth" Take Leading Roles at SIAM CSE Conference, June 2013, K. Willcox and H.-P. Langtangen
  - CSE 2013: Large-scale Network Analysis at SIAM CSE Conference, June 2013, T. Kolda and A. Pinar
  - CSE 2013: Navigating the Paths to a Career in CSE, June 2013, A. Davis
  - CSE 2013: Quantum Mechanics Without Wavefunctions, June 2013, M. Reuter and L.-W. Wang
  - CSE 2013: Taming Snakes and Dragons in the Earth, June 2013, A. Malcolm and A. Fichtner
  - CSE 2013: A Conference Within a Conference for MOR Researchers, July/Aug 2013, D. Amsallem, B. Haasdonk, and G. Rozza
  - CSE 2013: Cardiac Modeling: The Road from Equations to the Clinic, July/Aug 2013, N. Trayanova
  - CSE 2013: How Will the Fast Multipole Method Fare in the Exascale Era?, July/Aug 2013, L. Barba and R. Yokota

  Additional CSE-related articles in recent issues of SIAM News include:
  - Top Ten Reasons To Not Share Your Code (and why you should anyway), April 2013, R. LeVeque
  - The Remarkable Career of a Pioneering Computational Scientist, Nov 2013, G. Pieper and L.C. McInnes
  - The 2013 Nobel Prize in Chemistry Celebrates Computations in Chemistry and Biology, Dec 2013, T. Schlick

- SciDAC: Accelerating Scientific Discovery, Transforming Computational Science, April 2014, E. D'Azevedo, E. Ng, S. Wild

- **SIAM Review.** Recent CSE-related articles in SIAM Review include:
  - Making Do with Less: An Introduction to Compressed Sensing, K. Bryan and T. Leise, SIAM Rev. 55-3 (2013), pp. 547-566
  - Global Convergence of Radial Basis Function Trust-Region Algorithms for Derivative-Free Optimization, S. Wild and C. Shoemaker, SIAM Rev. 55-2 (2013), pp. 349-37

7. What activities are planned and proposed for the next period of the charter? Please describe scheduled and suggested future activities in detail.

Plans for the CSE15 conference are underway. The conference co-chairs are Hans De Sterck, Chris Johnson, and Lois Curfman McInnes, and the conference will be held in Salt Lake City from March 14-18, 2014 (www.siam.org/meetings/cse15/). The organizing committee and invited speakers represent an interdisciplinary mix of computational science expertise, including applied mathematics, computer science, and domain sciences.

For the first time, the CSE conference will be held in a convention center, which will enable us to handle potential conference growth in 2015 (with growth from ~800 to ~1300 participants from CSE11 to CSE13) and to absorb some SIAM activities that are normally held at the annual meeting but will shift to CSE15 because 2015 is an ICIAM year. Special activities at CSE15 include celebrating the 15th anniversary of SIAM-CSE conferences; increased emphasis on poster sessions, including demos, thematic groups of posters, and new poster prizes; increased profile of the awards ceremony; featured minisymposia in six thematic areas; and minitutorials related to the two special conference themes (CSE software and big data analytics). The CSE conference series is on a very successful track, with significant growth in participation over the past years. The goals of the new conference elements described above are (1) to raise the profile of poster presentations as a mechanism to handle potential conference growth (with poster blitzes and poster sessions as part of the daytime program), and (2) to provide conference attendees with additional rallying points (featured minisymposia, minitutorials) in addition to the traditional minisymposia and invited plenary talks.

An outcome of the Aug 2014 CSE Workshop on Future Directions in CSE Education and Research will be a draft document discussing these issues. We will present this draft document at CSE15 and request feedback from the community.

A future consideration may be establishing an early-career CSE award as a complement to the existing (senior) SIAM/ACM Prize in CSE.

8. How can SIAM help the activity group achieve its goals?

SIAM can best help the CSE community by continuing to promote CSE and to encourage increased funding from federal agencies that traditionally have had difficulty supporting the interdisciplinary research that is essential to CSE. CSE methods and competence are becoming increasingly relevant for scientists in fields other than mathematics. These include physics, chemistry, computer science and various engineering disciplines, to name just a few. SIAM should consider strategies to attract more members from these disciplines and integrate them under the CSE umbrella.

9. How can the activity group help SIAM in its general role of promoting applied mathematics and computational science?

SIAM continues to be the professional society for CSE. Applied mathematics is integral to the community and continues to grow. This SIAG is a medium for professionals to gain information about trends and the cutting edge of research through the CSE conference series and mailing list. As more subfields continue to emerge in CSE, we anticipate that SIAM's membership base and breadth will correspondingly expand. The CSE SIAG will continue to foster research in new areas and to support growth in related subfields. Moreover, this multidisciplinary SIAG will expose a wide range of professionals to applied mathematics.

As encouraged by the prior SIAG CSE charter renewal, the SIAG is now taking an active role in identifying directions for future CSE education and research. The SIAG could also take a more active role in promoting academic activity as far as curriculum and trends. A CSE education subgroup could be well served to help direct specific issues to the SIAM Education committee, as CSE will continue to be an area of growth in colleges and universities.

This SIAG requests that the SIAM Council and Board of Trustees renew its charter for a two year operating period beginning January 1, 2015.

Signed,

Uli Ruede, SIAG/CSE Chair
May 21, 2014